GEORGIA INSTITUTE OF TECHNOLOGY OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ______

Project No. G-35-672 (R6161-0A0) GTRC/~~GIT~~ DATE 7 / 8 /86

Project Director: Robert P. Lowell School/~~Lab~~ Geophysical Sciences

Sponsor: Georgia Department of Natural Resources

Type Agreement: Contract No. 701-690351 dated 6/11/86

Award Period: From 6/11/86 To ~~6/10/87~~ 9/10/87 (Performance) 6/10/87 (Reports)

Sponsor Amount:

	This Change	Total to Date
Estimated:	$ 7,390	$ 7,390
Funded:	$ 7,390	$ 7,390

Cost Sharing Amount: $ 169 Cost Sharing No: G-35-369 (F6161-0A0)

Title: Research on Contaminant Transport in Fractured Rock

ADMINISTRATIVE DATA

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Defense Priority Rating: N/A

Military Security Classification: N/A
(or) Company/Industrial Proprietary: N/A

RESTRICTIONS

See Attached N/A Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval – Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with none proposed or anticipated.

COMMENTS:

JUL 1986 RECEIVED SUPPORT SERVICES OCA

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GEORGIA INSTITUTE OF TECHNOLOGY **OFFICE OF CONTRACT ADMINISTRATION**

2-47
SR-1

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date: 10-22-87

Project No. G-35-672

School/~~Lab~~ Geophysical Sciences

Includes Subproject No.(s) N/A

Project Director(s) Robert P. Lowell GTRC / ~~GIT~~

Sponsor Georgia Department of Natural Resources

Title Research on Contaminant Transport in Fractured Rock

Effective Completion Date: 9-10-87 (Performance) 9-10-87 (Reports)

Grant/Contract Closeout Actions Remaining:

- [ ] None
- [x] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [x] Final Report of Inventions -- Sent Questionaire to P. I.
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other

Continues Project No. Continued by Project No.

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FORM OCA 69.285

G-35-672

CONTAMINANT TRANSPORT IN FRACTURED ROCK

Quarterly Report No. 1

Contract No. 701--690351

submitted to

Georgia Department of Natural Resources

by

Robert P. Lowell

School of Geophysical Sciences

Georgia Institute of Technology

Date: September 11, 1986

Introduction

In the past few years there has been much more attention devoted to modeling of fluid flow and contaminant transport in fractured rock. Models have been both analytical and numerical, and are generally constructed on the idea of dual-porosity as proposed by Barenblatt et al. (1960). In this approach, matrix blocks of relatively high porosity and low permeability are separated by a fracture network of low porosity and high permeability. Thus the main fluid transport is through the fractures, while the matrix blocks act as sources or sinks of fluid for the fractures. In problems focusing on contaminant transport, the matrix blocks act as sinks for the contaminant; that is, contaminant bearing fluid is advected through the fractures while the contaminant is diffused into the matrix. Among the recent analytical treatments are those of Tang et al. (1981), Sudicky and Frind (1982), and Rasmussen (1984). Some numerical models based on the finite element method have been developed by Huyakorn et al. (1983a,b). The analytical models treat the case of contaminant transport in a single fracture, or a set of parallel fractures, imbedded in an infinite porous rock matrix. Flow through the fractures is uniform, isothermal and one-dimensional. The concentration of contaminant is assumed to be continuous across the fracture-matrix interface. The concentration at the inlet to the fracture is assumed to be constant.

In the research being performed under this contract, several modifications are being made to the ultra-simple models that have been developed. Here models are being developed for contaminant transport in a single fracture in which: (1) the inlet concentration of the contaminant is a harmonic function of time; (2) the contaminant is injected into a horizontal sub-surface fracture from a point source; (3) the groundwater velocity is a function of time; (4) the concentration of contaminant is discontinuous across the fracture-matrix interface. In this report items (1) and (2) are discussed. Items (3) and (4) will be the subject of later reports.

Basic Equations

In the models developed here, the basic equations for contaminant transport in the fracture and matrix will be taken from Tang et al. (1981). The equation for the matrix, where transport is by diffusion only, is

$$\partial c'/\partial t = (D'/R')\partial^2 c'/\partial z^2 - \lambda c' \qquad b < z \leq \infty \tag{1}$$

where c' is the concentration in the matrix, D' is the molecular diffusivity in the matrix, R' is the retardation factor, and λ is the decay constant for the radioactive species. The cartesian coordinate z is directed perpendicularly to the fracture, and the fracture width is $2b$. The corresponding equation for the fracture, where transport is by dispersion and advection, is

$$\partial c/\partial t + (v/R)\partial c/\partial x = (D/R)\partial^2 c/\partial x^2 - \lambda c + (\theta D'/bR)\partial c'/\partial z\Big|_{z = b} \qquad (2)$$

where c′ is the concentration of the contaminant in the fracture, v the average velocity in the fracture, R the retardation factor in the fracture, and D the longitudinal dispersion coefficient. The cartesian coordinate x is directed along the fracture plane. The last term in (2) couples the concentration in the matrix to the concentration in the fracture. At the interface z = b, c = c′. Equation (2) serves as a boundary condition to (1) at the fracture interface.

Initial conditions and a boundary condition at the inlet x = 0 are also required. In this paper it is assumed that

$$c = c' = 0 \quad \text{at } t = 0 \quad \text{(no initial contaminant)} \qquad (3)$$

At the inlet to the fracture, two conditions will be treated.

$$c = c_o \exp(i\omega t) \qquad (4a)$$

so that the inlet condition is a harmonic function of time; and

$$c = c_o \qquad (4b)$$

where c_o is a constant. Tang _et al._ (1981) treated the problem given by equations (1) through (3), with condition (4b). In this report, some results using condition (4a) are derived. In addition, some calculations in which a point source of contaminant is injected into s subsurface, horizontal fracture are performed.

Results

A. Inlet concentration a harmonic function of time.

The problem is given by equations (1) through (3), with condition (4a). The solution derived here is for the steady oscilllatory solution, the initial transient is ignored. The oscillatory solution can be found by substituting solutions of the form

$$c' = c_o \exp(i\omega t + mx + n(z - b))$$

and

$$c = c_o \exp(i\omega t + mx)$$

into (1) and (2) respectively. One then obtains for n and m:

$$n = (R'/D')^{1/2}(i\omega + \lambda)^{1/2} \tag{5}$$

$$m = \left[v/R \pm (v^2/R^2 - 4(D/R)(-(i\omega + \lambda) + \theta D'n/bR))^{1/2}\right]/(2D/R) \tag{6}$$

Because n and m are complex numbers, the form of the solution is that of a damped traveling wave. The skin depth and phase speed are complicated factors, however, and considerable insight can be gained by making some simplyifing approximations. For example, one can ask whether dispersion in the fracture is important comaperd to advection. If the ratio $vL/D \gg 1$, where L is an appropriate scale length, then dispersion can be neglected. This ratio can be evaluated by using the numerical parameters of Tang et al. (1981). They write:

$$D = \alpha v + D^* \tag{7}$$

where $\alpha = 0.5$m is the dispersivity and $D^* = 1.6 \times 10^{-9} m^2 s^{-1}$. For v in the range 10^{-6}--$10^{-7} ms^{-1}$, $D \sim \alpha v$; and the criteria for whether dispersion can be neglected becomes $L/\alpha \gg 1$. The appropriate scale length L for the problem at hand is the skin depth δ. Because dispersion in the fracture tends to increase the skin depth, an approximate result can be obtained by estimating δ when D = 0. Then:

$$m = -(R/v)(\lambda + i\omega) + (\theta D'/bv)(R'/D')^{1/2}(\omega^2 + \lambda^2)^{1/4}$$

$$\cdot(\cos(\hat{\theta} + 2\pi)/2 + i\sin(\hat{\theta} + 2\pi)/2)) \tag{8}$$

where $\hat{\theta} = \tan^{-1}(\omega/\lambda)$. Consider further the special cases of $\lambda \ll \omega$ and $\lambda \gg \omega$.

1. the case $\lambda \ll \omega$.

If $\lambda \ll \omega$, $\hat{\theta} \sim \pi/2$ and (8) reduces to

$$m = -iR\omega/v - (\theta/bv)(R'\omega D'/2)^{1/2}(1 + i) \tag{9}$$

and the skin depth is given by

$$\delta = (bv/\theta)(2/R'\omega D')^{1/2} \tag{10}$$

To evaluate δ, consider the parameter values given below. They are approximately the same as used by Tang et al. (1981)

$b = 10^{-3}$--10^{-4}m

$\theta = 0.01$

$R = R' = 1.0$

$D' = 10^{-10} m^2 s^{-1}$

$\omega = 6 \times 10^{-5} s^{-1}$ (diurnal oscillation)

$\omega = 2 \times 10^{-8} s^{-1}$ (yearly oscillation)

The velocity v is in the range used previously. Substituting these parameters into (10) yields $1.7 \times 10^{-2} < \delta < 10^{2}$, where the small δ value is for the diurnal oscillation in a narrow fracture having a low flow velocity; and the large value of δ is for the yearly oscillation in a wider fracture with a higher flow velocity. As a general rule, one can neglect disperison in systems where the contaminant input oscillates on an annual basis.

2. the case $\lambda >> \omega$.

In this case $\hat{\theta}$ in (8) is nearly zero, and m reduces to

$$m = -(R/v)(i\omega + \lambda) - (\theta/bv)(RD'\lambda)^{1/2} \tag{11}$$

There are now two decay terms:

$$\delta_1 = v/R \tag{12}$$

and

$$\delta_2 = (bv/\theta)(RD'\lambda)^{-1/2} \tag{13}$$

For any case of interest, in which $\lambda >> \omega$, the discussion is restricted to the situation where $\omega = 2 \times 10^{-8} s^{-1}$. As an example, suppose $\lambda = 2 \times 10^{-7} s^{-1}$ (i.e. $T_{1/2} = 3 \times 10^{6}$s). Then the ratio of equation (12) to equation (13) is

$$\delta_1/\delta_2 = (\theta/bR)(R'D'/\lambda)^{1/2} \tag{14}$$

For the parameters used previously, $\delta_1/\delta_2 = 2.2$, if $b = 10^{-3}$m and $\delta_1/\delta_2 = 0.22$ if b = 10-4m. The result is independent of the flow velocity. Thus for the case $\lambda >> \omega$ and wide fractures, loss to the matrix is more important than radioactvie decay in the fracture; whereas for narrow fractures, radioactive decay is a more important loss mechanism than diffusion into the matrix.

B. Point Source Injection into a Fracture.

The problem is to investigate the transport of a contaminant in a single horizontal fracture as a result of input from an injection well. The regional groundwater flow is negligible comapared to the rate of fluid injection, and the contaminant is assumed to move radially away from the well. Transport of contaminant in the matrix is still given by (1), but because of the cylindrical symmetry of the problem, the equation governing transport in the fracture is modified. The new equation is:

$$\partial c/\partial t + (Q/2\pi rb)\partial c/\partial r = (D/Rr)\partial(r\partial c/\partial r)/\partial r - \lambda c$$
$$+ (\theta D'/bR)\partial c'/\partial z\Big|_{z = b} \qquad (15)$$

where r is the distance from the axis of the well.

The solution to (1) and (15) is found, subject to conditions (3) and (4b) using the method of Laplace transforms. The analysis is similar to that of Tang et al. (1981). The solution is exceptionally cumbersome when dispersion in the fracture is included. The equation for transport in the fracture in Laplace transform space is a form of Bessel's equation of non-integral order. For the sake of simplicity, solutions are obtained for the limiting case of no dispersion ($D = 0$). Then the solution to (15) in Laplace transform space that satisfies (4b) is:

$$\bar{c} = (c_o/p)\exp\left[-(\pi br^2/Q)(p + \lambda)\right]\exp(-Ar^2(p + \lambda)^{1/2}) \qquad (16)$$

where $\bar{c}$ is $\mathcal{L}(c)$ and $A = (R'D')^{1/2}(\theta/bR)$. The inverse Laplace transform of (16) gives the contaminant concentration in the fracture. The result is:

$$c/c_o = 0 \qquad \tau < 0$$

$$c/c_o = (1/2)\exp(-\pi br^2\lambda/Q)\left[\exp(-Ar^2\lambda^{1/2})\mathrm{erfc}(Ar^2/2\tau^{1/2} - (\lambda\tau)^{1/2})\right.$$
$$\left. + \exp(Ar^2\lambda^{1/2})\mathrm{erfc}(Ar^2/2\tau^{1/2} + (\lambda\tau)^{1/2})\right] \qquad \tau \geq 0 \quad (17)$$

where erfc is the complementary error function and $\tau = t - \pi br^2/Q$. As $\tau \to \infty$, (17) approaches the steady state solution

$$c/c_o = \exp\left[-(\pi b\lambda/Q + (R'D'\lambda)^{1/2}(\theta/bR))r^2\right] \qquad (18)$$

As a sample calculation, using (18), suppose $Q = 10^{-3} m^3 s^{-1}$, $b = 10^{-3} m$, $\lambda = 1.8 \times 10^{-9} s^{-1}$ (appropriate for tritium), and the other parameters as used previously. Substitution of numerical values into (18) yields

$$c/c_o = \exp(-(0.56 + 4.2) \times 10^{-8} r^2) \qquad (19)$$

where the first number in the exponential function is the numerical value of the first term in the exponent in (18) and the second number is the numerical value of the corresponding term in (18). Equation (19) shows that for the decay constant chosen loss to the matrix is much more important than decay of the isotope in the fracture. If the fluid injection rate were higher or the fracture were narrower, the relative importance of the two terms would be even more preonounced. From equation (19), the concentration would fall to 1% of the initial concentration at approximately 10km from the well. Thus the contaminant would affect a considerable area. It is for this reason that measures are taken to restrict movement of the contaminant-bearing fluid that is disposed of by subsurface injection.

Future Research

Succeeding reports will treat the problem of a varying fluid flow in the fracture and the problem of forming a skin on the fracture-matrix interface so that the concentration in the matrix and fracture are discontinuous at the interface.

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CONTAMINANT TRANSPORT IN FRACTURED ROCK

Quarterly Report No. 2

Contract No. 701--690351

submitted to

Georgia Department of Natural Resources

by

Robert P. Lowell

School of Geophysical Sciences

Georgia Institute of Technology

Date: December 11, 1986

Introduction

In this quarterly report the problem of contaminant transport in a fracture that develops a fracture-skin is investigated. Physically, this condition corresponds to the situation in which diffusion from the fracture to the surrounding rock matrix is inhibited. Mathematically, the condition means that the concentration in the fracture and matrix is not continuous. The boundary condition at z = b then takes the form:

$$\theta D' \partial c'/\partial x|_{x=b} = H(c'-c)|_{x=b} \qquad (1)$$

where H is a parameter, analogous to a heat transfer coefficient, that represents the effect of the fracture skin. If H is large, the results revert to the situation in which the fracture-skin is absent.

Basic Equations

The basic transport equations for contaminant in the fracture and the matrix are equations (1) and (2) respectively of Report No. 1. They are reproduced here for convenience.

In the matrix:

$$\partial c'/\partial t = (D'/R')\, {}^2 c'/\partial z^2 - \lambda c' \qquad b < z \leq \infty \qquad (2)$$

where c' is the concentration in the matrix, D' is the molecular diffusivity in the matrix, R' is the retardation factor, and λ is the decay constant for the radioactive species. The cartesian coordinate z is directed perpendicularly to the fracture, and the fracture width is 2b.

In the fracture:

$$\partial c/\partial t + (v/R')\partial c/\partial x = (D/R)\partial^2 c/\partial x^2 - c + (\theta D'/bR)\partial c/\partial z|_{z=b} \qquad (3)$$

where c is the concentration of the contaminant in the fracture, v the average velocity in the fracture, R the retardation factor in the fracture, and D the longitudinal dispersion coefficient. The cartesian coordinate x is directed along the fracture plane. The last term in (3) couples the concentration in the matrix to the concentration in the fracture. At the interface z = b, c = c'. Equation (3) serves as a boundary condition to (2) at the fracture interface.

In addition to condition (1), the other conditions are:

$$c'(x,z,0) = c(x,0) = 0 \qquad \text{(no initial contaminant)} \qquad (4)$$

and

$$c(0,t) = c_0 \qquad \text{(a constant concentration } c_0 \text{ at the inlet)} \qquad (5)$$

Solution

Following Tang et al. (1981), equations (1) through (5) are solved using Laplace Transforms. In Laplace transform space, the solution to (2) is exactly as given by Tang et al. (1981). Equation (3) becomes, after using (1),

$$\partial^2\bar{c}/\partial x^2 - (v/D)\partial\bar{c}/\partial x - (R/d)(P + (\theta D'/bR)(BHP^{1/2}/(H - B\theta DP^{1/2}))\bar{c} = 0 \quad (6)$$

where $\bar{c}$ is the Laplace transform of c and $P = p + \lambda$. Note that for large H equation (6) reduces to the corresponding equation in Tang et al. (1981).

a) special case $H < < 1$.

If H is small, the fracture-skin strongly inhibits diffusion into the matrix. In this case, (6) reduces to:

$$\partial^2\bar{c}/\partial x^2 - (v/D)\partial\bar{c}/\partial x - (R/D)(p + \lambda^*)\bar{c} = 0 \quad (7)$$

where $\lambda^* = \lambda - H/bR$. The solution to equation (7), with condition (5) is found to be:

$$\bar{c} = (c_0 g)\exp(v/2D - P^{1/2})x/(P-a) \quad (8)$$

where

$$a = (v/2D)^2 + R\lambda^* D$$

$$g = R/D$$

The inverse transform can be found by standard techniques. The result is:

$$c/c_0 = (1/2)\exp(vx/2D)[\exp(-a^{1/2}x)\mathrm{erfc}(x/2(Dt/R)^{1/2}-(aDt/R)^{1/2})$$
$$+ \exp(a^{1/2}x)\ \mathrm{erfc}\ (x/2(Dt/R)^{1/2} + (aDt/R)^{1/2})] \quad (9)$$

b) Special case $D = 0$, $H < < 1$.

If one neglects dispersion in equation (6), then the resulting solution in Laplace transform space is:

$$\bar{c}/c_0 = \exp(-RPx/v)\ \exp(-\theta D'BP^{1/2}H\ x/bR(H-P^{1/2}B\theta D'))/P-\lambda) \quad (10)$$

For large H, this solution reduces to the corresponding case treated by Tang, <u>et al.</u> (1981). For small H, (10) reduces to

$$\bar{c}/c_0 = \exp((H/bR - R\lambda/v)x)\ \exp(-Rpx/v)/p \quad (11)$$

thus

$$c/c_0 = \exp((H/bR-R\lambda/v)x \quad \text{for } t>Rx/v \quad (12)$$

Solutions (9) and (12) show that the effect of the fracture-skin is to confine the contaminant to the fracture. In fact D', the diffusion coefficient in the matrix, does not even enter into the solution. The importance of these results in any practical situation will require a thorough study of the rock characteristics, particularly along fracture interfaces, to see whether a fracture-skin exists, and whether it is effective in inhibiting loss of the contaminant to the rock matrix.

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Tang, D. H., E. O. Frind, and E. A. Sudicky (1981). Contaminant transport in fractured porous media: Analytical solutions for a single fracture, Water, Res. Research, 17, 555-564.

G-35-672

CONTAMINANT TRANSPORT IN FRACTURED ROCK

Quarterly Report No. 3

Contract No. 701--690351

submitted to

Georgia Department of Natural Resources

by

Robert P. Lowell
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Atlanta, Georgia 30332

Date: March 10, 1987

Introduction

In this quarterly report, the problem of contaminant transport in a fracture in which the flow is a harmonic function of time is treated. This is a rather realistic phenomenon in natural systems because many locales have seasonal variations of water input into the ground water system (e.g., spring snow melt and/or rain). The solution to this problem follows from that derived in Quarterly Report #1. In that report, the flow was assumed to be constant. The case of oscillating flow is treated as a perturbation on the steady flow case in a manner analogous to Bodvarsson (1969).

The analysis given below represents a completion of the four tasks that were required under this contract. The final report, a draft of which will be delivered by May 10, 1987, will represent a synthesis of the three quarterly reports.

Basic Equations

The basic transport equations for contaminant in the fracture and in the matrix are equations (1) and (2) of Quarterly Report #1. They are reproduced here for convenience.

In the matrix:

$$\partial c'/\partial t = (D'/R')\partial^2 c'/\partial z^2 - \lambda c' \quad b < z \le \infty \tag{1}$$

where c' is the concentration in the matrix, D' is the molecular diffusivity in the matrix, R' is the retardation factor, and λ is the decay constant for the radioactive species. The cartesian coordinate z is directed perpendicularly to the fracture, and the fracture width is $2b$.

In the fracture:

$$\partial c/\partial t + (v/R)\partial c/\partial x = (D/R)\partial^2 c/\partial x^2 - \lambda c + (\theta D'/bR)\partial c'/\partial z|_{z=b} \tag{2}$$

where c is the concentration of the contaminant in the fracture, v the average velocity in the fracture, R the retardation factor in the fracture and D the longitudinal dispersion coefficient. The cartesian coordinate x is directed along the fracture plane. The last term in (2) couples the concentration in the matrix to the concentration in the fracture. At the interface $z = b$, $c = c'$. Equation (2) serves as a boundary condition to (1) at the fracture interface.

The initial boundary conditions are:

$$c'(x,z,0) = c(x,0) = 0 \qquad \text{(no initial contaminant),} \tag{3}$$

$$c(0,t) = c^{o} e^{i\omega t} \quad \text{(an oscillatory concentration } c^{o} \text{ at the inlet)} \tag{4}$$

and

$$c(x,t) = c'(x,b,t) \tag{5}$$

(the concentration across the matrix fracture interface is continuous)

Solution

As noted in Quarterly Report #1, dispersion generally can be neglected in flow when the period of oscillation is yearly. For simplicity, D will be set equal to zero in the following analysis. One now supposes that the velocity v in the fracture is a periodic function of time and that the amplitude of the velocity fluctuations is small compared to the mean flow. Then

$$v = v_{o}(1+v^{*}\cos(\omega^{*}t+\phi)) \tag{6}$$

where $|v^{*}| << 1$ and ϕ is an arbitrary phase angle. Within this form for the velocity field in (2), the problem can be solved by a perturbation method. That is, let

$$c' = c_{o}' + c_{1}' \text{ and } c = c_{o} + c_{1} \tag{7}$$

where c_{o} and c_{o}' are the "zeroth" order solutions for when the velocity is constant and c_{1}' and c_{1} are first order perturbation quantities. Upon substituting (6) and (7) into (1) and (2) and equating terms of like order and neglecting products of first order perturbation terms as second order (hence small), one obtains

$$\partial c_o'/\partial t = (D'/R')\partial^2 c_o'/\partial z^2 - \lambda c_o' \tag{8}$$

$$\partial c_1'/\partial t = (D'/R')\partial c_1'/\partial z^2 - \lambda c_1' \tag{9}$$

$$\partial c_o/\partial t + (v_o/R)\partial c_o/\partial x = -\lambda c_o + (\theta D'/bR)\partial c_o'/\partial z|_{z=b} \tag{10}$$

$$\partial c_1/\partial t + (v_o/R)\partial c_1/\partial x + (v_o v^*/R)\cos(\omega^* t+\phi)\ c_o/\partial x = -\lambda c_1 + (\theta D'/bR)\partial c_1'/\partial z|_{z=b} \tag{11}$$

Equations (8) and (10) are the zeroth order equations for which solutions have been obtained in Quarterly Report #1. Equations (9) and (11) are the first order perturbation equations. Equation (9) is identical in form to (8), but in (11) an additional term appears. This term, the last one on the left of (11), acts as a source term for the c_1 equation. Since c_o is known, this source term can be written explicitly. From the previous work, where $v = v_o$, a constant, c_o is given by

$$c_o = c^o \exp(i\omega t + mx) \tag{12}$$

where $m = -(R/v_o)(\lambda + i\omega) + (\theta D'/v_o b)(R'/D')^{1/2}(\lambda + i\omega)^{1/2}$ (13)

Thus, (11) can be written

$$\partial c_1/\partial t + (v_o/R)\partial c_1/\partial x = -\lambda c_1 + (\theta D'/bR)(\partial c_1/\partial z)|_{z=b} - (c^o v_o v^* m/R)\cos(\omega^* t+\phi)\exp(i\omega t + mx) \tag{14}$$

In the formulation that follows, the algebra becomes exceedingly cumbersome. Moreover, relatively rapid flow velocities will be considered so that the transport terms in (10) and (11) are much greater than the inertial terms (Bodvarsson, 1969). For the sake of convenience, λ is set equal to zero. The complex number in (13) and (14) becomes a little easier to deal with:

$$m = -\alpha(1 + i) \tag{15}$$

where $\alpha = (\theta D'/bv_o)(\omega R'/2D')^{1/2}$ and $i = \sqrt{-1}$

Upon writing the complex number m in polar terms,

$$m = -(\alpha)e^{-\pi/4}$$

and recognizing that the physical solutions to (14) involve only the real parts of (12) and (14), the source term in (14) can be written

$$G = A\{\cos[(\omega+\omega^*)t - \alpha x - \pi/4 + \phi] + \cos[(\omega - \omega^*)t - \alpha x - \pi/4 - \phi]\}\exp(-\alpha x) \tag{16}$$

where $A = c^o \ v_o v^*/2R$

With the above simplifications, one can write the first order perturbation equations (9) and (11)

$$\partial c_1'/\partial t = (D'/R')\partial^2 c_1'/\partial z^2 \tag{17}$$

$$(v_o/R)\partial c_1/\partial x = (\theta D'/bR)\partial c_1'/\partial t|_{z=b} + G \tag{18}$$

Equations (17) and (18) are subject to the homogeneous initial conditions and c_1 must satisfy a homogeneous condition on the inlet $x = z = 0$.

Following Bodvarsson (1969), solutions to (17) and (18) are expressed as S = P + H where P is a particular solution and H is a general solution with the source term absent in (19).

For a general source term $G = Ae^{-\alpha x}\cos(wt - \alpha x + \gamma)$ where $w = \omega + \omega^*$, one assumes a solution to (17) of the form.

$$c_1^1 = A_1\exp(-\alpha x - \gamma(z-b)) \cos(wt - \alpha x - \gamma(z-b) + \psi) + \tag{19}$$

$$A_2\exp(-\alpha x - \gamma(z-b))\sin(wt - \alpha x - \gamma(z-b) + \psi)$$

Upon substituting (19) into (17) one finds

$$\gamma = (wR'/2D')^{1/2} \tag{20}$$

Upon substituting (19) into (18) and setting z = b, one obtains

$$A_1 = A_2 = \frac{A}{2(\theta/bR)(R'D'/2)^{1/2}(w^{1/2}-\omega^{1/2})} \tag{21}$$

The particular solution for c_1 is found by setting z = b in (19).For the above derived expression of c_1, one must add a solution H to the homogeneous equation that is chosen to satisfy the boundary condition $c_1(0,t)=0$. This solution is found to be

$$H = A_1\exp(-px - \gamma(z-b))\cos(wt-px-\gamma(z-b)+\psi) + \tag{22}$$

$$A_1\exp(-px-\gamma(z-b)\sin(wt-px-\gamma(z-b)+\psi)$$

$$\text{where } p = \alpha(w/\omega)^{1/2} \tag{23}$$

The solution to the perturbation equation for c_1 consists of the sum of solutions, P-H, where P is (19) with z = b , is given by (20), and A_1 and A_2 given by (21); and H is given by (22) with p given by (23). the complete solution in values the sum P-H for $w = \omega + \omega^*$ and $w = \omega - \omega^*$. Thus the final result is

$$c_1(x,t) = \left(\frac{c^o v^*}{4}\right)\left(\frac{1/2}{(\omega+\omega^*)^{1/2} - \omega^{1/2}}\right)\Big\{ e^{-\alpha x}[\cos((\omega+\omega^*)t - \alpha x + \phi - 3\pi/4) + \tag{24}$$

$$\sin((\omega+\omega^*)t - \alpha x + \phi - 3\pi/4)] - e^{-\alpha\left(\frac{\omega+\omega^*}{\omega}\right)^{1/2}}[\cos((\omega+\omega^*)t - \alpha\left(\frac{\omega+\omega^*}{\omega}\right)^{1/2} x + \phi - 3\pi/4) +$$

$$\sin((\omega+\omega^*)t - \alpha\left(\frac{\omega+\omega^*}{\omega}\right)^{1/2} x + \phi - 3\pi/4)]\Big\}$$

$$\left(\frac{c^o v^*}{4}\right)\left(\frac{\omega^{1/2}}{|(\omega-\omega)^{1/2})| - \omega^{1/2}}\right)\Big\{ e^{-\alpha x}[\cos((\omega-\omega^*)t - \alpha x + \phi - 3\pi/4) + \sin((\omega-\omega^*)t - \alpha x + \phi - 3\pi/4)\}$$

$$-e^{-\alpha x}\left(\left|\frac{\omega+\omega^*}{\omega}\right|\right)^{1/2}[\cos(\omega+\omega^*)t - \alpha\left|\frac{(\omega-\omega^*)}{\omega}\right|^{1/2} x - \phi - 3\pi/4) + \sin(\omega-\omega^*)t - \alpha\left|\frac{(\omega-\omega^*)}{\omega}\right|^{1/2} x - \phi - 3\pi/4]\Big\}$$

The perturbed contaminant distribution c_1, due to the oscillatory flow thus consists of a fast mode ($\omega + \omega^*$) and a slow mode ($\omega - \omega^*$). The slower mode has a larger amplitude; the maximum amplitude occurs at $\omega = \omega^*$. Such a resonance condition is typical in such oscillatory systems.

The resonance condition may be of some practical interest since the frequency of injections of contaminant and the frequency of oscillation in gorundwater flow velocity may both occur on a yearly basis. In the case $\omega = \omega^*$, the final term in square brackets dominates the perturbation for if $\omega = \omega^*$, both the time dependence and x dependence vanish.

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Some Analytical Models for

Contaminant Transport In Fractured Rock

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Final Report

Georgia Geologic Survey Contract No.701--690351

September, 1987

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Introduction

The characterization of how various contaminants are transported in ground-water systems is certainly one of the most important problems in ground-water hydrology today. This characterization is based largely on spatial and temporal data that delineate the extent of contamination, define physical parameters and describe the flow regime; but it is also important to have sound physical and mathematical concepts of the transport process in order to predict the future advance of the contaminant and to devise appropriate cleanup measures. Mathematical models can be divided into two general types: analytical models and numerical models. With analytical models, the transport equations and boundary conditions are solved in functional form. To do this, many assumptions and simplifications are often made regarding the details of the transport processes in order to make the mathematics tractable. The solutions found by this method are therefore to be considered first order approximations. Such solutions represent important first steps in the analysis of a potential contaminant transport problem because they can provide valuable insights regarding the physics of the phenomena and the relative importance of various parameters. Analytical models are especially valuable in areas where the data base is limited. On the other hand, in situations where a well-documented problem exists, and a wealth of data is available, numerical models may be appropriate in order to model the contaminant transport problem in detail. Numerical models have their own set of deficiencies. In most cases it is not possible to rigorously verify that the solutions obtained are correct. Often one argues for the validity of a numerical scheme because it gives the correct answer to a problem for which an analytical solution has been obtained. It is therefore useful to have a number of analytical solutions against which numerical models can be checked.

Analytical models are the focus of this paper. It is particularly important to develop models of contaminant transport in rock formations in which the dominant permeability derives from a network of discrete fractures. Fracture permeability undoubtedly best describes the rock formations of the Georgia Piedmont and in many other locales as well. In order to begin to appreciate the importance of fracture permeability on contaminant transport, a number of idealized problems relating to transport in a single discrete fracture will be developed.

Related Work

In the past few years there has been much more attention devoted to modeling of fluid flow and contaminant transport in fractured rock. Models have been both analytical and numerical, and are generally constructed on the idea of dual-porosity as proposed by Barenblatt et al. (1960). In this approach, matrix blocks of relatively high porosity and low permeability are separated by a fracture network of low porosity and high permeability. Thus the main fluid transport is through the fractures, while the matrix blocks act as sources or sinks of fluid for the fractures. In problems focusing on contaminant transport, the matrix blocks act as sinks for the contaminant; that is, contaminant bearing fluid is advected through the fractures while it is diffused into the matrix. Among the recent analytical treatments are those of Neretnieks (1980), Tang et al. (1981), Sudicky and Frind (1982), and Rasmuson (1984). Some numerical models based on the finite element method have been developed by Huyakorn et al. (1983a,b); and some experimental, laboratory scale modeling, has also been performed (Sudcicky et al., 1985; Starr et al., 1985).

The analytical models mentioned above make a variety of assumptions. For the purposes of this paper, Tang et al. (1981) serves as the starting point. They treat the case of contaminant transport in a single, discrete fracture, represented as a thin infinite sheet,, imbedded in an infinite porous rock matrix. The flow through the fracture is uniform, one-dimensional and isothermal. The concentration of contaminant is assumed to be continuous across the fracture-matrix interface. The concentration of contaminant at the inlet to the fracture is assumed to be uniform in space and time. A schematic of the idealized system geometry is shown in Figure 1. In this paper, a number of modifications will be made to the ultra-simple analytical model of Tang et al. (1981). These include: (1) a treatment of the effect of a "fracture skin", i. e., an interface between the fracture surface and the rock matrix that acts to inhibit diffusion of the contaminant into the matrix; (2) an analysis of a problem in radial flow; (3) a consideration of the effect of the contaminant concentration at the inlet as a periodic function of time; and (4) a treatment of the ground-water flow as a periodic function of time.

Basic Equations

In the models developed here, the basic equations for contaminant transport in the fracture and matrix will be taken from Tang et al. (1981). The equation for the matrix, where transport is by diffusion only, is

$$\delta c'/\delta t = (D'/R')\delta^2 c'/\delta z^2 - \mu c' \qquad b < z \leq \infty \qquad (1)$$

where c' is the concentration in the matrix, D' is the molecular diffusivity in the matrix, R' is the retardation factor, and μ is the decay constant for the radioactive species. The cartesian coordinate z is directed perpendicularly to the fracture, and the fracture width is $2b$. The symbols used in this paper are given in the List of Symbols. The corresponding equation for the fracture, where transport is by dispersion and advection, is:

$$\delta c/\delta t + (v/R)\delta c/\delta x = (D/R)\delta^2 c/\delta x^2 - \mu c + (\theta D'/bR)\delta c'/\delta z \Big|_{z=b} \qquad (2)$$

where c is the concentration of the contaminant in the fracture, v the average velocity in the fracture, R the retardation factor in the fracture, θ the porosity of the matrix, and D the longitudinal dispersion coefficient. The cartesian coordinate x is directed along the fracture plane. The last term in (2) couples the concentration in the matrix to the concentration in the fracture. At the interface z = b, c = c'. Equation (2) serves as a boundary condition to (1) at the fracture interface.

Initial conditions and a boundary condition at the inlet x = 0 are also required. In this paper it is assumed that

$$c = c' = 0 \quad \text{at } t = 0 \quad \text{(no initial contaminant)} \qquad (3)$$

At the inlet to the fracture, two conditions will be treated:

$$c = c^{o}\exp(i\sigma t) \qquad (4a)$$

so that the inlet condition is a harmonic function of time ($i = (-1)^{\frac{1}{2}}$; and

$$c = c^{o} \qquad (4b)$$

where c^{o} is a constant. Tang <u>et al.</u> (1981) treated the problem given by equations (1) through (3), with condition (4b). In this paper, new results are derived that entail modifications to these basic equations.

Results

A. The Effect of a Fracture Skin

In this section the problem of contaminant transport in a fracture that develops a fracture-skin is investigated. A somewhat analogous problem has been treated by Moench (1984). Physically, this condition corresponds to the situation in which diffusion from the fracture to the surrounding rock matrix is inhibited. Mathematically, the condition means that the concentration in the fracture and matrix is not continuous. The boundary condition at z = b then takes the form:

$$\theta D'\delta c'/\delta x \Big|_{z=b} = H(c'-c)\Big|_{z=b} \qquad (5)$$

where H is a parameter, analogous to a heat transfer coefficient, that represents the effect of the fracture skin. If H is large, the results revert to the situation in which the fracture-skin is absent.

Following Tang <u>et al.</u> (1981), equations (1) through (3) along with (4b) and (5) are solved using Laplace Transforms. In Laplace transform space, the solution to (1) for the contaminant concentration in the matrix is exactly as given by Tang <u>et al.</u> (1981). Since the primary interest in this analysis is the contaminant concentration in the fracture, this solution will not be reproduced here. Equation (2) becomes, after using (5),

$$\delta^2 C/\delta x^2 - (v/D)\delta C/\delta x -$$

$$(R/D)(P + (\Theta D'/bR)(BHP^{\frac{1}{2}}/(H + B\Theta D'P^{\frac{1}{2}}))C = 0 \qquad (6)$$

where C(x,p) is the Laplace transform of c, $B = (R'/D')^{\frac{1}{2}}$, and $P = p + \mu$. Note that for large H equation (6) reduces to the corresponding equation in Tang <u>et al.</u> (1981).

a) special case H < < 1.

If H is small, the fracture-skin strongly inhibits diffusion into the matrix. In this case, (6) reduces to:

$$\delta^2 C/\delta x^2 - (v/D)\delta C/\delta x - (R/D)(p + \mu^*) = 0 \qquad (7)$$

where $\mu^* = \mu + H/bR$. The solution to equation (7), with condition (4b) is found to be:

$$C = (c^O g)\exp[(v/2D - P^{\frac{1}{2}})x]/(P-a) \qquad (8)$$

where

$$a = (v/2D)^2 + R\mu^* D$$

$$g = R/D$$

The inverse transform can be found by standard techniques. The result is:

$$c/c^O = (1/2)\exp(vx/2D)[\exp(-a^{\frac{1}{2}}x)\mathrm{erfc}(x/2(Dt/R)^{\frac{1}{2}} - (aDt/R)^{\frac{1}{2}})$$

$$+ \exp(a^{\frac{1}{2}}x)\ \mathrm{erfc}(x/2(Dt/R)^{\frac{1}{2}} + (aDt/R)^{\frac{1}{2}})] \qquad (9)$$

b) Special case D = 0, H < < 1.

If one neglects dispersion in equation (6), then the resulting solution in Laplace transform space is:

$$C/c^{o} = \exp(-RPx/v)\ \exp[-\theta D'BP^{\frac{1}{2}}H\ x/bR(H + P^{\frac{1}{2}}B\theta D')]/(P - \mu) \qquad (10)$$

For large H, this solution reduces to the corresponding case treated by Tang, et al. (1981). For small H, (10) reduces to

$$C/c^{o} = \exp[-(H/bR + R\mu/v)x]\exp(-Rpx/v)/p \qquad (11)$$

thus

$$c/c^{o} = \exp[-(H/bR + R\mu/v)x] \qquad \text{for } t > Rx/v \qquad (12)$$

Solutions (9) and (12) show that the effect of the fracture-skin is to confine the contaminant to the fracture. In fact D', the diffusion coefficient in the matrix, does not even enter into the solution. The importance of these results in any practical situation will require a thorough study of the rock characteristics, particularly along fracture interfaces, to see whether a fracture-skin exists, and whether it is effective in inhibiting loss of the contaminant to the rock matrix.

B. Point Source Injection into a Fracture.

In some cases, the contaminant laden fluid is not injected into the ground along a line as was the case in Tang et al. (1981) and in the preceding example. Rather the contaminant is disposed of by injecting it into a borehole; the contaminant then spreads radially away from the borehole. Because of its fundamental importance in ground-water pollution, there exists a considerable literature on radial flow in a porous aquifer. Hoopes and Harleman (1967) consider the problem of two-dimensional radial flow from an injection well, but they neglect diffusive losses from the aquifer. Dagan (1971) used singular asymptotic expansions to obtain solutions for hydrodynamic dispersion in radial flow. Tang and Babu (1979) used the method of Laplace transforms to obtain approximate solutions of the radial dispersion equation, but they neglected diffusion from the aquifer to the surrounding rock matrix as well as radioactive decay of the contaminant, as, for example, in the case of a tritium tracer. Chen (1985) treats the problem of radial flow from an injection well including diffusive losses from the main aquifer into to adjacent strata of low permeability. He uses the Laplace transform method to develop solutions that are valid for early times and approximately valid for large times. He does not include radioactive decay of the contaminant in this paper. Chen (1986) does include radioactive decay and he develops a steady state as well as approximate solutions valid for short times. He also argues that longitudinal dispersion becomes less important with longer injection times, and that the steady state solution without dispersion ought to be valid.

In this section a solution is derived for radial flow of contaminant from a injection well. The problem developed here is essentially identical to that of Chen (1986), except that the emphasis of the discussion will be somewhat different. As in Chen (1985, 1986), the regional ground-water flow is assumed to be negligible compared to the rate of fluid injection, the contaminant is assumed to move radially away from the well, and the rate of injection is assumed to uniform. Transport of contaminant in the matrix is still given by (1), and the initial condition by (3), but because of the cylindrical symmetry of the problem, the equation governing transport in the fracture is modified. Equation (2) is replaced by:

$$\delta c/\delta t + (Q/2\pi rbR)\delta c/\delta r = (1/Rr)(\delta(rDc)/\delta r)/\delta r - \mu c + (\theta D'/bR)\delta c'/\delta z\Big|_{z=b} \qquad (13)$$

where r is the distance from the axis of the well and Q is the rate of injection of the fluid into the well in m^3/s.

Approximate solutions to (1) and (13), subject to conditions (3) and (4b) (applied at r = 0 rather than x = 0), using the method of Laplace transforms have been found by Chen (1986). The solution is exceptionally cumbersome when dispersion in the fracture is included. The equation for transport in the fracture in Laplace transform space is a form of Bessel's equation of non-integral order. For the sake of simplicity, therefore, solutions are obtained for the limiting case of no dispersion, D = 0. The numerical results of Chen (1986) show that this approximation is valid in the steady state, and rather simple dimensional analysis shows that it is a valid approximation as long as one considers large distances from the borehole. Then the solution to (13) in Laplace transform space that satisfies the initial and boundary conditions is:

$$C(r,p) = (c^o/p)\exp[-(\pi br^2/Q)(p + \mu)]\exp[-Sr^2(p + \mu)^{\frac{1}{2}}] \qquad (14)$$

where $S = (R'D')^{\frac{1}{2}}(\theta/bR)$. The inverse Laplace transform of (14) gives the contaminant concentration in the fracture. The result is:

$$c/c^o = 0 \qquad T < 0$$

$$c/c^o = (1/2)\exp(-\pi br^2\mu/Q)\ \{\exp(-Sr^2\mu^{\frac{1}{2}})\mathrm{erfc}(Sr^2/2T^{\frac{1}{2}} - (\mu T)^{\frac{1}{2}})$$
$$+ \exp(Sr^2\mu^{\frac{1}{2}})\mathrm{erfc}(Sr^2/2T^{\frac{1}{2}} + (\mu T)^{\frac{1}{2}})\} \qquad T \geq 0 \qquad (15)$$

where erfc is the complementary error function and $T = t - \pi br^2/Q$. As T approaches infinity, (15) approaches the steady state solution

$$c/c^o = \exp[-(\pi b\mu/Q + (R'D'\mu)^{\frac{1}{2}}(\Theta/bR))r^2] \qquad (16)$$

Figures 2a and 2b depict solutions of (16) as a function of Q for two values of the fracture half-width b and for $\mu = 1.8 \times 10^{-9}$/s. This value of μ is appropriate for tritium. The other parameters are as listed in Table 1. Figure 2a shows that for a fracture half-width of 10^{-4} m and a flow rate of only 10^{-7} m^3/s the concentration of contaminant is 0.1 of the inlet concentration at a distance greater than 0.5 km. from the source. For greater flow rates the rate of decay is considerably slower; appreciable levels of contaminant are found several kilometers downstream from the source. Figure 2b is the same as Figure 2a except that the fracture half-width is 10^{-3} m. A comparison of Figures 2a and 2b shows that wider fractures tend to inhibit downstream transport of contaminant for a given fluid injection rate. This result arises because the first term in the exponential in equation (16) is the dominant one. That is, in the steady state, decay of contaminant in the fracture is more important than diffusion into the rock matrix, for the decay constant chosen. In the absence of radioactive decay, i. e., $\mu = 0$, equation (15) reduces to:

$$c/c^o = \mathrm{erfc}(Sr^2/2T^{\frac{1}{2}})$$

This result is analogous to the result for radial transport of heat away from an injection well (Bodvarsson, 1972).

C. Inlet concentration a harmonic function of time.

One of the principal assumptions that has been made in the work of Tang et al. (1981) and others who have worked on the contaminant transport problem is that the concentration of contaminant at the inlet to the aquifer is constant in time. In reality, the contaminant is often injected episodically. One can readily envision the case in which contaminant is injected cyclically on either a daily or an annual basis. Solutions to the contaminant transport problem in which the inlet condition on the concentration is a periodic function of time are therefore useful. The periodic solutions obtained below will also serve as a test for numerical models as well as for laboratory and field tests. The analogous problem of temperature oscillations in a fluid flowing in fracture has been treated by Bodvarsson (1969). The problem is given by equations (1) through (3), with condition (4a). The solution derived here is for the steady oscillatory solution, the initial transient is ignored. The oscillatory solution can be found by substituting solutions of the form:

$$c' = c^o \exp(i\sigma t + mx + n(z - b))$$

and

$c = c^o \exp(i\sigma t + mx)$ into (1) and (2) respectively. One then obtains for n and m:

$$n = (R'/D')^{\frac{1}{2}}(i\sigma + \mu)^{\frac{1}{2}} \tag{17}$$

$$m = [v/R \pm (v^2/R^2 - 4(D/R)(-(i\sigma + \mu) + \theta D'n/bR))^{\frac{1}{2}}]/(2D/R) \tag{18}$$

Because n and m are complex numbers, the form of the solution is that of a damped traveling wave. The skin depth and phase speed are complicated factors, however, and considerable insight can be gained by making some simplifying approximations. For example, one can ask whether dispersion in the fracture is important compared to advection. If the ratio $vL/D >> 1$, where L is an appropriate scale length, then dispersion can be neglected. This ratio can be evaluated by using the numerical parameters of Tang et al. (1981). They write:

$$D = \alpha v + D^* \tag{19}$$

where $\alpha = 0.5$m is the dispersivity and the molecular diffusivity $D^* = 1.6 \times 10^{-9} m^2 s^{-1}$. For v in the range from 10^{-6} to $10^{-7} ms^{-1}$, $D \approx \alpha v$; and the criteria for whether dispersion can be neglected becomes $L/\alpha >> 1$. The appropriate scale length L for the problem at hand is the skin depth τ. Because dispersion in the fracture tends to increase the skin depth, an approximate result can be obtained by estimating τ when D = 0. Then:

$$m = -(R/v)(\mu + i\sigma) + (\theta/bv)(R'D')^{\frac{1}{2}}(\sigma^2 + \mu^2)^{\frac{1}{4}}$$

$$\cdot \{\cos[(\Omega + 2\pi)/2] + i \sin[(\Omega + 2\pi)/2]\} \tag{20}$$

where $\Omega = \tan^{-1}(\sigma/\mu)$. Consider further the special cases of $\mu << \sigma$ and $\mu >> \sigma$.

1. the case $\mu << \sigma$.

If $\mu << \sigma$, $\Omega \approx \pi/2$ and (20) reduces to

$$m = -iR\sigma/v - (\theta/bv)(R'\sigma D'/2)^{\frac{1}{2}}(1 + i) \tag{21}$$

and the skin depth is given by

$$\tau = (bv/\theta)(2/R'\sigma D')^{\frac{1}{2}} \tag{22}$$

Figures 3a and 3b depict how τ varies as a function of fracture half-width for different values of the flow rate and frequency σ. The fixed parameters are given in Table 1. They are the same values used by Tang et al. (1981) Figure 3a shows that for the annual variation and large velocity, dispersion is negligible at essentially all fracture widths; for small velocities dispersion only becomes negligible when the fracture width is of the order of 10^{-3} m. Figure 3b depicts the same calculation as Figure 3a except that it corresponds to the daily variation. Figure 3b shows that dispersion is important for essentially the entire range of fracture widths and velocities considered. The calculations indicate that dispersion will be important in laboratory and short term field models in which a periodic injection of contaminant is used where the frequency of injection is on a diurnal or higher frequency cycle.

2. the case $\mu >> \sigma$.

In this case Ω in (20) is nearly zero, and m reduces to

$$m = -(R/v)(i\sigma + \mu) - (\theta/bv)(R'D'\mu)^{\frac{1}{2}} \tag{23}$$

There are now two decay terms:

$$\tau_1 = v/R\mu \tag{24}$$

and

$$\tau_2 = (bv/\theta)(R'D'\mu)^{-\frac{1}{2}} \tag{25}$$

The ratio of equation (24) to equation (25) is:

$$\tau_1/\tau_2 = (\theta/bR)(R'D'/\mu)^{\frac{1}{2}} \tag{26}$$

Equation (26) for the ratio of the two skin depths is plotted as a function of fracture half-width for two different values of the decay constant. Figure 4 shows that provided that $b > 2 \times 10^{-4}$, $\tau_2 > \tau_1$. Thus the downstream penetration of contaminant is controlled by diffusion into the matrix and not simply by radioactive decay in the fracture. This result is independent of the flow rate in the fracture.

D. Time-Varying Flow in the Fracture

Another assumption that has been made in all analytical treatment of contaminant transport in fractures is that the flow rate of the ground water is constant in space and time. It is a common occurrence that ground-water flow varies as a function of time. In regions in which the aquifers are replenished in spring because of snow melt and/or seasonal rains one would expect the ground-water flow rate to vary on an annual basis. If the contaminant input is also time-varying there may be resonance effects that lead to enhanced transport. The problem of a time-varying flow rate is treated below by using a perturbation method.

As noted above, dispersion generally can be neglected in flow when the period of oscillation of the contaminant input is yearly. For simplicity, D will be set equal to zero in the following analysis. One now supposes that the velocity v in the fracture is a periodic function of time and that the amplitude of the velocity fluctuations is small compared to the mean flow. Then:

$$v = v_o(1+v^*\cos(\sigma^* t + \phi)) \qquad (27)$$

where $|v^*| << 1$ and ϕ is an arbitrary phase angle. With this form for the velocity field in (2), the problem can be solved by a perturbation method. That is, let

$$c' = c'_o + c'_1 \text{ and } c = c_o + c_1 \qquad (28)$$

where c'_o and c_o are the "zeroth" order solutions for when the velocity is constant and c'_1 and c_1 are first order perturbation quantities. Upon substituting (27) and (28) into (1) and (2), equating terms of like order, and neglecting products of first order perturbation terms as second order (hence small), one obtains:

$$\delta c'_o/\delta t = (D'/R')\delta^2 c'_o/\delta z^2 - \mu c'_o \qquad (29)$$

$$\delta c'_1/\delta t = (D'/R')\delta^2 c'_1/\delta z^2 - \mu c'_1 \qquad (30)$$

$$\delta c_o/\delta t + (v_o/R)\delta c_o/\delta x = -\mu c_o + (\Theta D'/bR)\delta c'_o/\delta z|_{z=b} \qquad (31)$$

$$\delta c_1/\delta t + (v_o/R)\delta c_1/\delta x + (v_o v^*/R)\cos(\sigma^* t + \phi)\delta c_o/\delta x = \qquad (32)$$

$$-\mu c_1 + (\Theta D'/bR)\delta c'_1/\delta z|_{z=b}$$

Equations (29) and (31) are the zeroth order equations for which solutions have been obtained in the previous section. Equations (30) and (32) are the first order perturbation equations.

Equation (30) is identical in form to (29), but in (32) an additional term appears. This term, the last one on the left of (32), acts as a source term for the c_1 equation. Since c_o is known, this source term can be written explicitly. From the previous work, where $v = v_o$, a constant, c_o is given by

$$c_o = c^o \exp(i\sigma t + mx) \tag{33}$$

where

$$m = -(R/v_o)(\mu + i\sigma) + (\theta/v_o b)(R'D')^{\frac{1}{2}}(\mu + i\sigma)^{\frac{1}{2}} \tag{34}$$

Thus, (32) can be written

$$\delta c_1/\delta t + (v_o/R)\delta c_1/\delta x = -\mu c_1 - (c^o v_o v^* m/R)\cos(\sigma^* t + \phi) \tag{35}$$

$$\cdot \exp(i\sigma t + mx) + (\theta D'/bR)(\delta c'_1/\delta z)|_{z = b}$$

In the formulation that follows, the algebra becomes exceedingly cumbersome. Moreover, relatively rapid flow velocities will be considered so that the transport terms in (31) and (32) are much greater than the inertial terms (Bodvarsson, 1969). For the sake of convenience, μ is set equal to zero. The complex number m in (34) and (35) becomes a little easier to deal with:

$$m = -\beta(1 + i) \tag{36}$$

where $\beta = (\theta/bv_o)(\sigma R'D'/2)^{\frac{1}{2}}$. Upon writing the complex number m in polar terms,

$$m = -\beta\exp(-\pi/4)$$

and recognizing that the physical solutions to (35) involve only the real parts of (33) and (35), the source term in (35) can be written:

$$G = A\{\cos[(\sigma + \sigma^*)t - \beta x - \pi/4 + \phi] + \tag{37}$$

$$\cos[(\sigma - \sigma^*)t - \beta x - \pi/4 - \phi]\}\exp(-\beta x)$$

where $A = c^o v_o v^*/2R$. With the above simplifications, one can write the first order perturbation equations (31) and (33):

$$\delta c'_1/\delta t = (D'/R')\delta^2 c'_1/\delta z^2 \tag{38}$$

$$(v_o/R)\delta c_1/\delta x = G + (\Theta D'/bR)\delta c_1/\delta t|_{z = b} \tag{39}$$

Equations (38) and (39) are subject to the homogeneous initial conditions and c_1 must satisfy a homogeneous condition on the inlet $x = z = 0$.

Following Bodvarsson (1969), solutions to (38) and (39) are expressed as the sum U + V where U is a particular solution and V is a general solution with the source term absent in (39). For a general source term $G = A\exp(-\beta x)\cos(wt - \beta x + \Phi)$ where $w = \sigma + \sigma^*$, one assumes a solution to (38) of the form.

$$c'_1 = A_1\exp(-\beta x - \epsilon(z-b))\ \cos(wt - \beta x - \epsilon(z-b) + \Phi) + \tag{40}$$

$$A_2\exp(-\beta x - \epsilon(z-b))\ \sin(wt - \beta x -\epsilon(z-b) + \Phi)$$

Upon substituting (40) into (38) one finds

$$\epsilon = (wR'/2D')^{\frac{1}{2}} \tag{41}$$

Upon substituting (40) into (39) and setting z = b, one obtains:

$$A_1 = A_2 = \frac{A}{2(\Theta/bR)(R'D'/2)^{\frac{1}{2}}(w^{\frac{1}{2}} - \sigma^{\frac{1}{2}})} \tag{42}$$

The particular solution U for c_1 is found by setting z = b in (40). For the above derived expression of c_1, one must add a solution V to the homogeneous equation that is chosen to satisfy the boundary condition $c_1(0,t) = 0$. This solution is found to be

$$V = A_1\exp[-sx - \epsilon(z-b)]\cos(wt - sx - \epsilon(z-b) + \Phi) + \tag{43}$$

$$A_1\exp[-sx - \epsilon(z-b)]\sin(wt - sx - \epsilon(z-b) + \Phi)$$

where

$$s = \beta(w/\sigma)^{\frac{1}{2}} \tag{44}$$

The solution to the perturbation equation for c_1 thus consists of the sum of solutions, U - V, where U is (40) with $z = b$, ϵ is given by (41), and A_1 and A_2 given by (42); and V is given by (43) with s given by (44). The complete solution involves the sum U - V for $w = \sigma + \sigma^*$ and $w = \sigma - \sigma^*$. Thus the final result is:

$$
\begin{aligned}
c_1(x,t) = {} & (c^o v^*/2)[\sigma^{\frac{1}{2}}/((\sigma + \sigma^*)^{\frac{1}{2}} - \sigma^{\frac{1}{2}})] \qquad (45) \\
& \cdot\{\exp(-\beta x)\cos((\sigma + \sigma^*)t - \beta x + \phi) \\
& - \exp[-((\sigma + \sigma^*)/\sigma)^{\frac{1}{2}}\beta x]\cos((\sigma + \sigma^*)t - \beta((\sigma + \sigma^*)/\sigma)^{\frac{1}{2}}x + \phi)\} \\
& + (c^o v^*/2)[\sigma^{\frac{1}{2}}/(|(\sigma - \sigma^*)^{\frac{1}{2}}| - \sigma^{\frac{1}{2}})] \\
& \cdot\{\exp(-\beta x)\cos((\sigma - \sigma^*)t - \beta x - \phi) \\
& - \exp[-((|\sigma - \sigma^*|)/\sigma)^{\frac{1}{2}}\beta x]\cos((\sigma - \sigma^*)t - \beta((|\sigma - \sigma^*|)/\sigma)^{\frac{1}{2}}x - \phi)\}
\end{aligned}
$$

The perturbed contaminant distribution c_1, due to the oscillatory flow thus consists of a fast mode $(\sigma + \sigma^*)$ and a slow mode $(\sigma + \sigma^*)$. The slower mode has a larger amplitude; the maximum amplitude occurs at $\sigma = \sigma^*$. Such a resonance condition is typical in such oscillatory systems.

The resonance condition may be of some practical interest since the frequency of injections of contaminant and the frequency of oscillation in groundwater flow velocity may both occur on a yearly basis. In the case $\sigma = \sigma^*$, the final term of (45) dominates the perturbation; for if $\sigma = \sigma^*$, both the time dependence and x dependence of that term vanish. This term will dominate the perturbation at large x, and the magnitude of the perturbation will be $c_1 = (c^o v^*/2) \cos(-\phi)$. If the velocity and contaminant injection cycles are in phase, i. e., $\phi = 0$, then at large x the perturbation to the contaminant concentration will be $c^o(v^*/2)$. That is there will be a d.c. transport of contaminant downstream in an amount that represents the initial concentration multiplied by one half of the magnitude of the velocity perturbation. This may be a significant effect.

Conclusions

This paper has been concerned with the development of analytical models for contaminant transport in a single, planar fracture. The models that have been derived have considered the effects of a fracture skin that inhibits the diffusion of contaminant into the porous rock matrix. If the skin is non-adsorbing, contaminant may be transported considerably further downstream than if the skin were absent. The models have also considered the phenomenon of radial transport of contaminant away from an injection well. The steady-state calculations showed that contaminant could be transported several kilometers downstream from the well, particularly in narrow fractures. This calculation also showed that radioactive decay in the fracture controlled the downstream penetration rather than diffusion into the rock matrix. Finally, models in which the source concentration and flow rate were periodic functions of time were developed. The calculations showed that dispersion could be neglected for long period oscillations (e.g. annual) but not for short period ones. For cases in which the radioactive decay constant was large compared to the inlet variation frequency, the skin depth was controlled by diffusion into the matrix. Resonance effects between contaminant input cycles and natural groundwater flow rate fluctuations could lead to enhanced downstream transport of contaminant. All of the analytical calculations may be useful for interpreting laboratory or field experiments of contaminant transport in fractured rock as well as for the verification of numerical codes.

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Table 1: Parameter Values

$\Theta = 0.01$
$R = R' = 1.0$
$D' = 10^{-9}\ m^2s^{-1}$

List of Symbols

Lower case:

a - symbol to denote a convenient parameter group, see equation (8)
b - fracture half-width
c - contaminant concentration in fracture
c' - contaminant concentration in rock matrix
c^o - contaminant concentration at fracture inlet
g - symbol to denote a convenient parameter group, see equation (8)
m - wavenumber in x direction for periodic solutions
n - wavenumber in z direction for periodic solutions
p - Laplace transform parameter
r - radial coordinate with reference to injection well
s - symbol to denote a convenient parameter group, see equation (44)
t - time
v - fluid flow velocity in fracture
v^* - perturbation velocity in fracture
w - $\sigma + \sigma^*$ or $\sigma - \sigma^*$
x - cartesian coordinate in direction of fluid flow
z - cartesian coordinate perpendicular to fracture/rock interface

Upper case:

A - amplitude factor in source term, see equation (37)
A_1, A_2 - amplitude factors in first order perturbation solutions, see equation (40)
B - symbol to denote a convenient parameter group, see equation (6)
C - Laplace transform of contaminant concentration
D - longitudinal dispersivity in fracture
D' - molecular diffusivity in rock matrix
D^* - molecular diffusivity of contaminant in fracture
G - source term in perturbation equation
H - fracture skin parameter (contaminant transfer coefficient)
L - scale length for neglect of dispersion (skin depth τ)
P - $p + \mu$
Q - volume fluid flow rate in injection well
R - retardation factor in fracture
R' - retardation factor in rock matrix
S - symbol to denote convenient parameter group, see equation (14)
T - symbol to denote convenient parameter group, see equation (15)
U - particular solution to perturbation differential equation
V - general solution to perturbation differential equation

Greek symbols:

α - dispersivity
β - symbol to denote convenient parameter group, see equation (36)
ϵ - symbol to denote convenient parameter group, see equation (41)
θ - porosity of matrix
μ - radioactive decay constant
μ^* - symbol to denote convenient parameter group, see equation (7)
σ - angular frequency of periodic contaminant input
σ^* - angular frequency of periodic flow velocity
τ - skin depth
ϕ - arbitrary phase angle
Φ - "general" phase angle in "general" source term
Ω - phase angle, see equation (20)

Subscripts:

o - refers to solution or parameter value for constant flow velocity
1 - refers to first order perturbation quantity

List of Figures

Figure 1. Schematic of a single fracture of width 2b imbedded in a rock matrix of low permeability.

Figure 2a. Steady-state contaminant concentration relative to the inlet concentration as function of radial distance from an injection well. b is the fracture half-width in meters. The legend refers to the volume flow rate Q in $m^3 s^{-1}$.

Figure 2b. Same as 2a except b = 0.001 m.

Figure 3a. Skin depth τ as a function of fracture width for two representative flow velocities in the fracture. v is the velocity in ms^{-1}. The value of σ corresponds to an annual periodicity in contaminant input.

Figure 3b. Same as 3a except σ corresponds to a diurnal periodicity.

Figure 4. Ratio of skin depths as a function of fracture width for periodic contaminant input in the case when the radioactive decay constant is much greater than the contaminant input frequency. Mu is the radioactive decay constant.

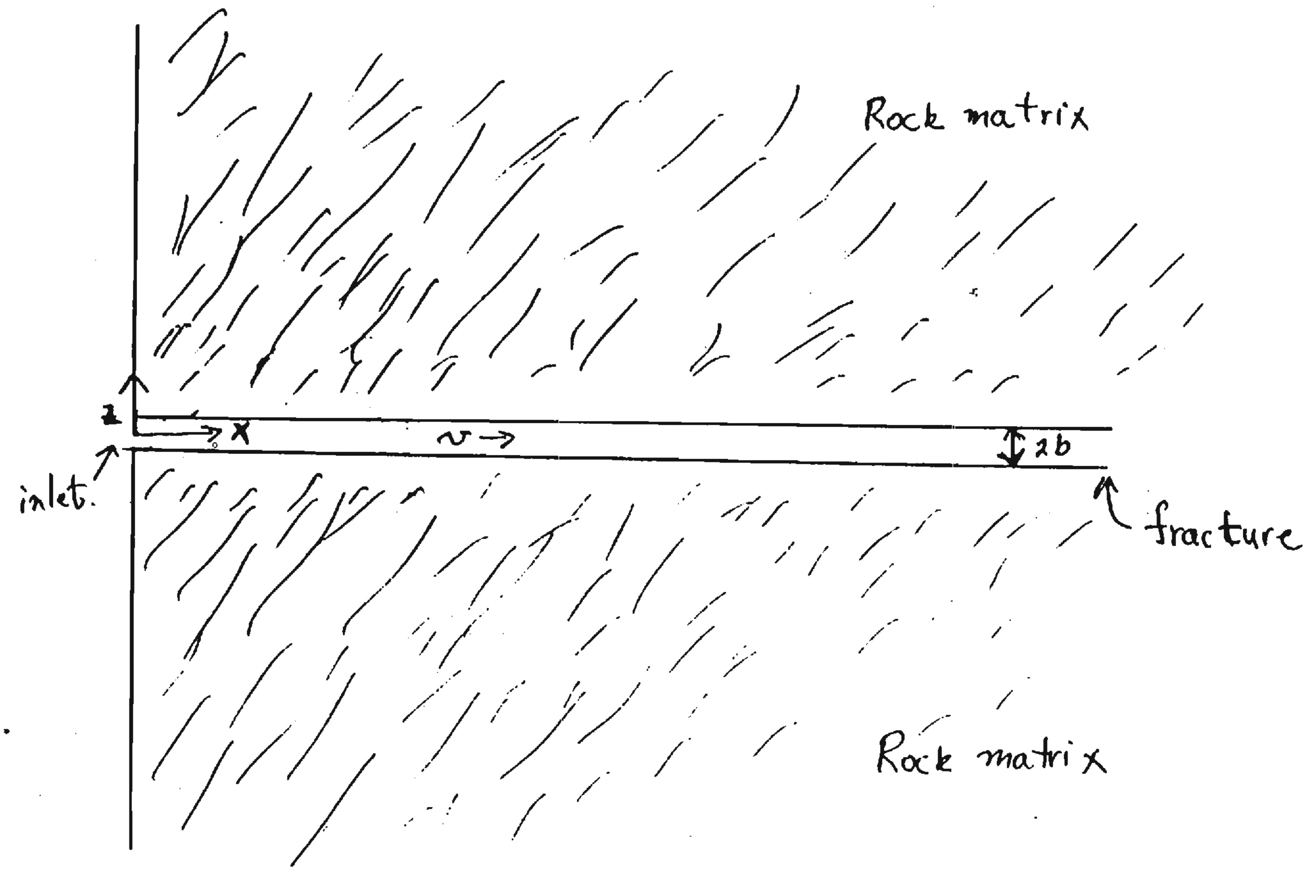


Figure 1

RADIAL CONTAMINANT TRANSPORT

b = .0001

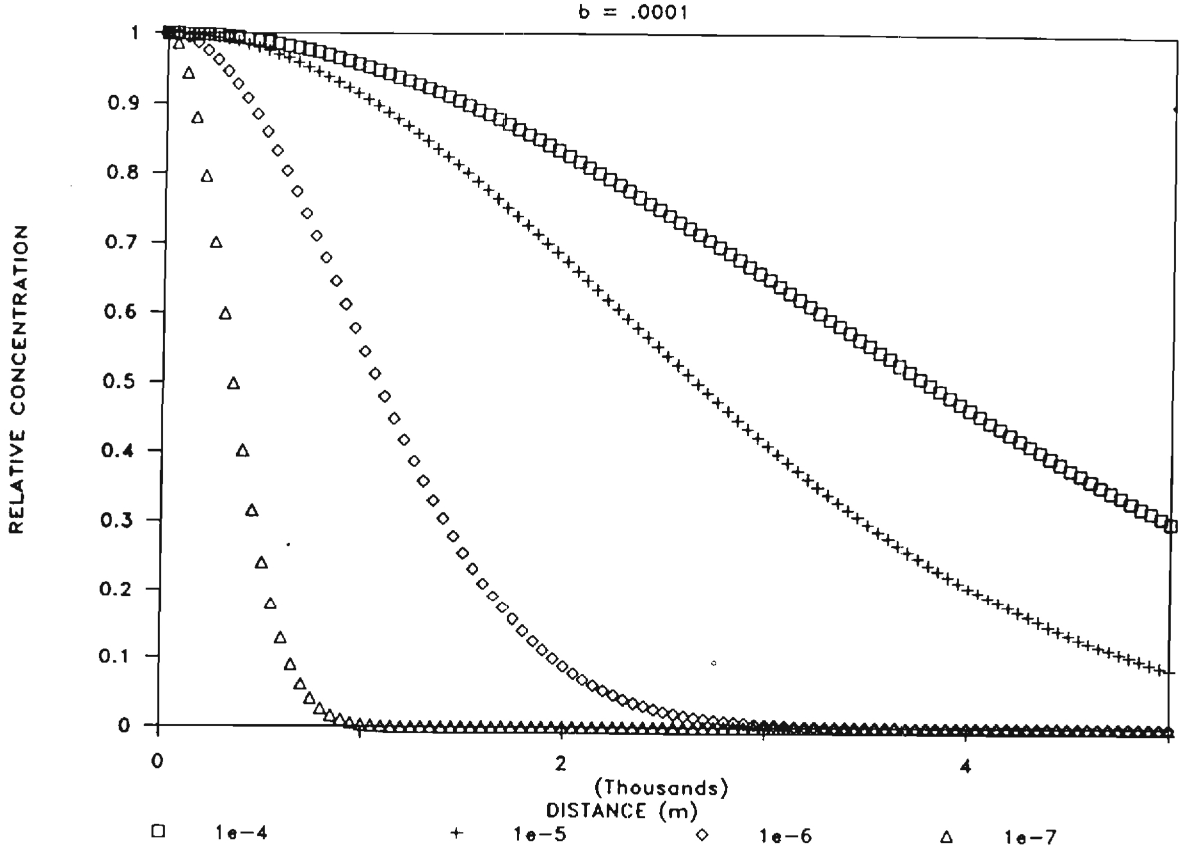
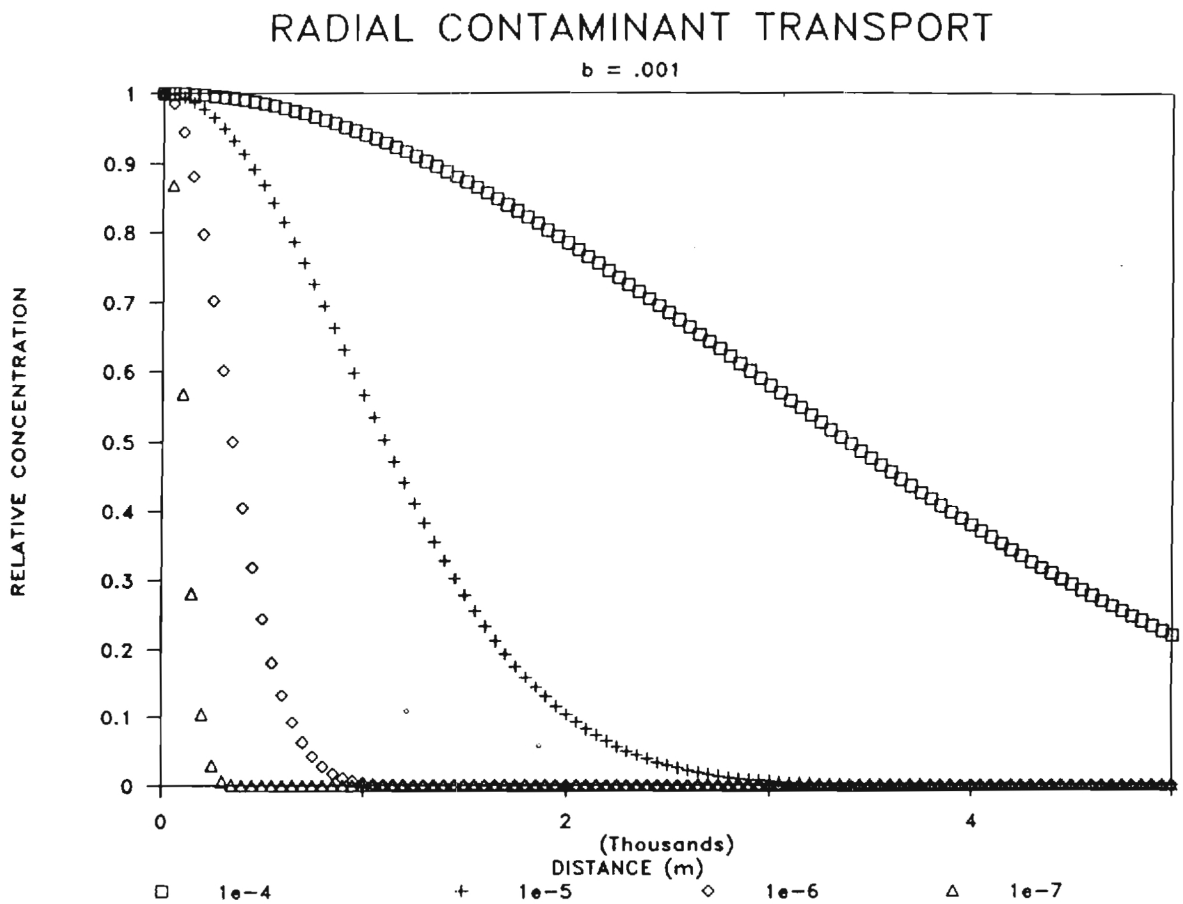
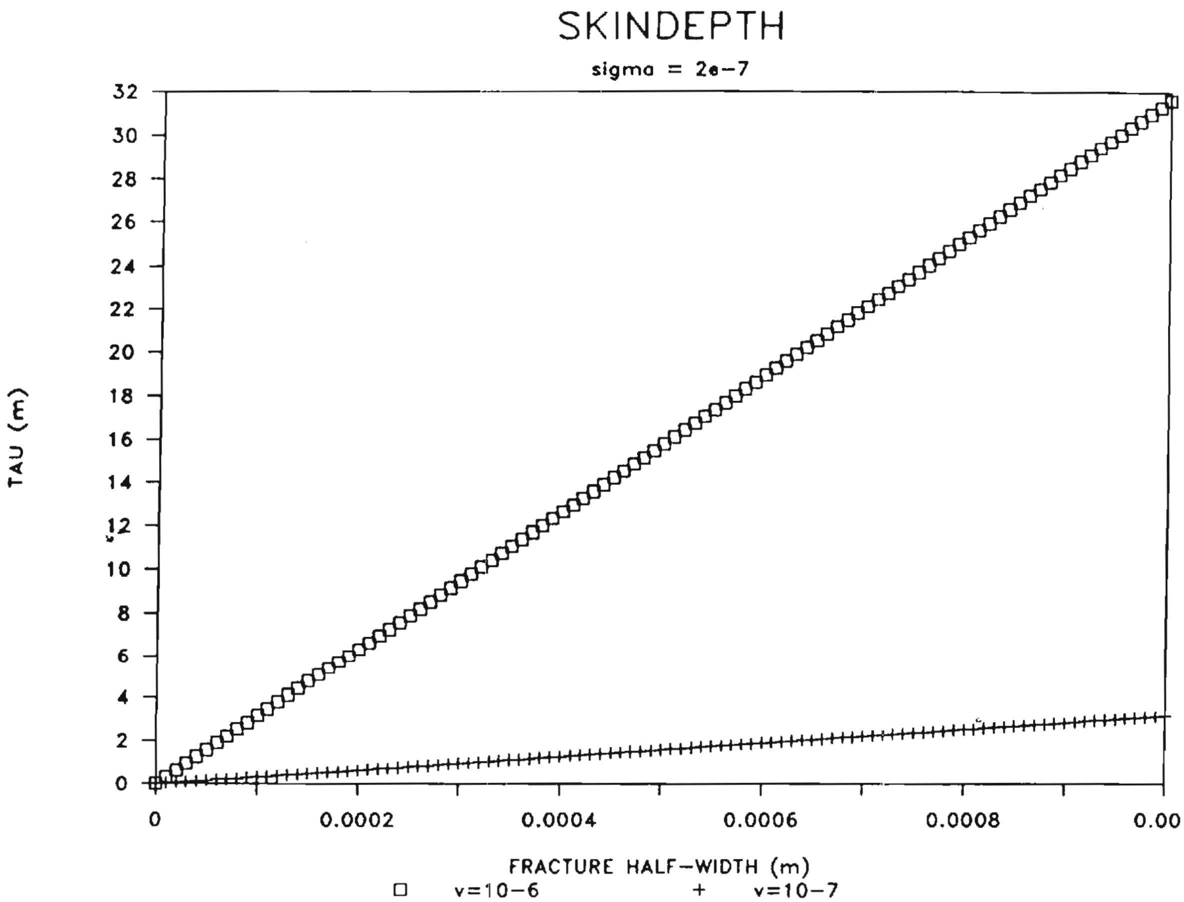
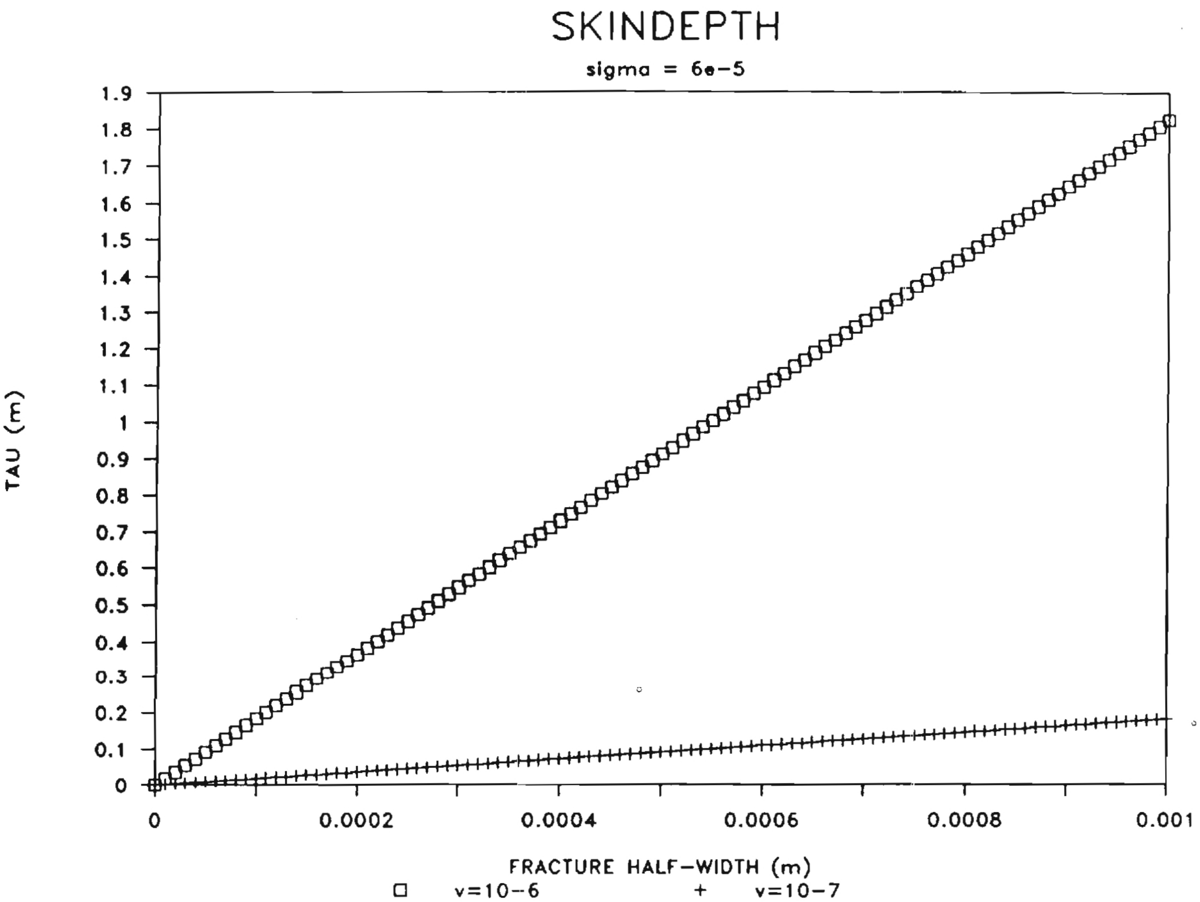


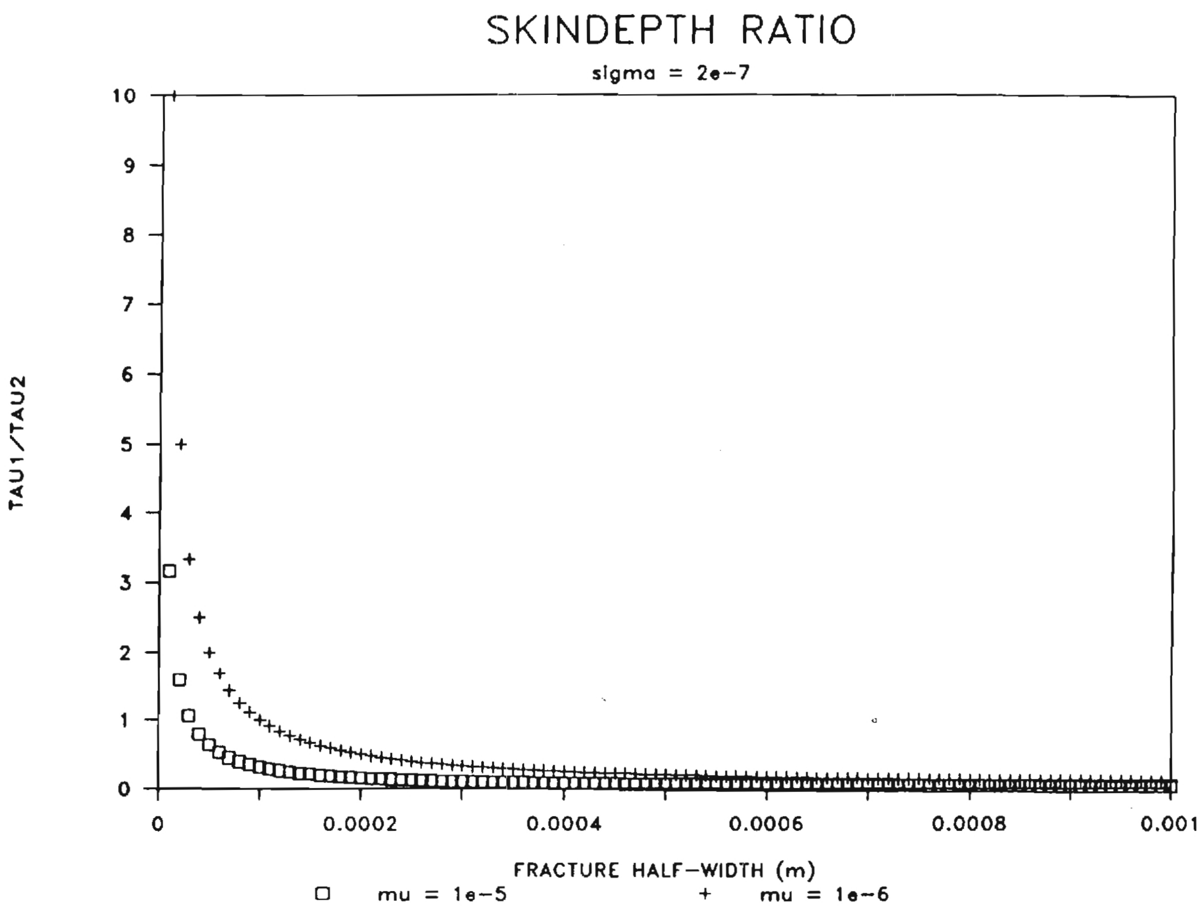
Fig 2a


RADIAL CONTAMINANT TRANSPORT
b = .001
RELATIVE CONCENTRATION
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
(Thousands)
DISTANCE (m)
1e-4
1e-5
1e-6
1e-7



SKINDEPTH
sigma = 2e-7
TAU (m)
32
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
0
0.0002
0.0004
0.0006
0.0008
0.001
FRACTURE HALF-WIDTH (m)
□ v=10-6
+ v=10-7


SKINDEPTH
sigma = 6e-5
TAU (m)
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.0002
0.0004
0.0006
0.0008
0.001
FRACTURE HALF-WIDTH (m)
v=10-6
v=10-7



SKINDEPTH RATIO
sigma = 2e-7
TAU1/TAU2
10
9
8
7
6
5
4
3
2
1
0
0
0.0002
0.0004
0.0006
0.0008
0.001
FRACTURE HALF-WIDTH (m)
mu = 1e-5
mu = 1e-6

1	28
2	29
3	30
4	
5	
6	
7	
8	
9	
10	
11	
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